Development of Advanced Metal–Organic Framework Materials: Synthesis, Characterization and Application Studies

SYNOPSIS

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UNIVERSITY DEPARTMENT OF CHEMISTRY

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FOR THE DEGREE OF

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BY

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B. N. MANDAL UNIVERSITY, LALOO NAGAR, MADHEPURA

SYNOPSIS OF RESEARCH WORK FOR Ph.D. DEGREE IN THE FACULTY OF SCIENCE (CHEMISTRY)

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INTRODUCTION

Metal–Organic Frameworks (MOFs) are an emerging class of crystalline porous materials constructed from metal ions/clusters coordinated to organic linkers. Their exceptionally high surface area, tunable porosity, functionalizable linkers, and structural modularity make them ideal for a variety of applications such as gas storage, catalysis, drug delivery, sensing, environmental remediation, and energy storage.

The design of MOFs allows precise control over topology, pore environment, and active sites. Synthetic strategies including solvothermal, mechanochemical, microwave-assisted, and diffusion methods enable fine modulation of framework geometry and chemical functionality. The proposed research aims to synthesize new MOFs through rational design of linkers and metal nodes, followed by detailed structural and physicochemical characterization and evaluation of their practical applications. This multidisciplinary work contributes significantly to coordination chemistry, materials science, and applied chemical research, similar in academic style to the sample synopsis

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Work Plan

a. Purpose and need of the study

The study is motivated by:

1. Increasing global demand for advanced porous materials for energy, environment, and biomedical applications.
2. MOFs offering unique tunability not accessible in traditional porous materials (zeolites, activated carbon).
3. Limitations in current MOF structures regarding stability, functionality, and application-

specific performance.

4. Need for systematic studies linking **synthetic modifications → structural features → real-world application**.
5. Continuous advancement in linker functionalization and metal-node engineering, which remains under-explored.

This research aims to contribute new knowledge in MOF synthesis, structure–property relationships, and functional applications.

Review of Literature of proposed work

This section will include:

1. Historical development, classification and chemistry of MOFs.
2. Synthetic methodologies: solvothermal, hydrothermal, sonochemical, microwave-assisted, electrochemical, mechanochemical.
3. Coordination behavior of linkers (carboxylates, pyridyl groups, imidazolates, phosphonates).
4. Crystal engineering principles: topology, metal secondary building units (SBUs), pore design.
5. Previous studies on MOF applications:
   • gas adsorption and separation
   • catalysis (Lewis acid, photocatalysis, redox catalysis)
   • drug delivery and biomedical uses
   • water purification and sensing
6. Challenges: structural stability, water tolerance, scalability, linker synthesis costs.
7. Recent advances in functionalized MOFs (mixed-linker, post-synthetic modification, flexible MOFs).

b. Details of the project with chapterization

Chapter- I: Introduction

Chapter- II: Survey of previous works

Chapter- III: Experimental

Chapter- IV: Result and Discussion

Chapter- V: Conclusion

Chapter I: Introduction

This chapter will provide an overview of background, significance, fundamentals of MOFs, overview of metal nodes and organic linkers.

Chapter II: Survey of Previous Works

This section will include:

- Historical development, classification and chemistry of MOFs.
- Synthetic methodologies: solvothermal, hydrothermal, sonochemical, microwave-assisted, electrochemical, mechanochemical.
- Coordination behavior of linkers (carboxylates, pyridyl groups, imidazolates, phosphonates).
- Crystal engineering principles: topology, metal secondary building units (SBUs), pore design.
- Previous studies on MOF applications:
    - gas adsorption and separation
    - catalysis (Lewis acid, photocatalysis, redox catalysis)
    - drug delivery and biomedical uses
    - water purification and sensing
- Challenges: structural stability, water tolerance, scalability, linker synthesis costs.

Recent advances in functionalized MOFs (mixed-linker, post-synthetic modification, flexible MOFs).

Chapter III: Experimental

This chapter will describe the Chemicals, synthesis of linkers, preparation of MOFs, characterization techniques.

Chapter IV: Results and Discussion

Structural analysis, spectroscopic interpretation, thermal stability, porosity measurements, and application performance.

Chapter V: Conclusion

This chapter will summarize the Summary, conclusions, and future scope.

c. Hypothesis

- Novel functionalized organic linkers can be designed to build MOFs with improved stability and tailored porosity.
- Using different metal ions (e.g., Zn^{2+}, Cu^{2+}, Co^{2+}, Zr^{4+}, Fe^{3+}) will allow generation of MOFs with distinct coordination geometries and topologies.
- The synthesized MOFs will show measurable enhancements in specific applications such as: gas storage/separation, catalytic activity, adsorption of pollutants and sensing
- Structure–property relationships can be established to correlate linker functionality, framework composition, and performance.

d. Methodology

Synthesis of Organic Linkers

- Designing aromatic carboxylate, pyridyl, or nitrogen-rich ligands.
- Multistep organic synthesis (condensation, substitution, functionalization).
- Purification by recrystallization or chromatography.

Synthesis of MOFs

1. **Solvothermal or hydrothermal synthesis** using metal salts and designed linkers.
2. **Alternative methods** such as sonochemical, microwave-assisted, or mechanochemical synthesis.
3. Optimization of parameters: metal-to-ligand ratio, temperature, pH, solvent system.

Characterization Techniques

- **FTIR**: confirmation of coordination and functional groups.
- **TGA/DSC**: thermal stability.
- **UV–Vis / Fluorescence**: optical properties (if applicable).
- **SEM/TEM**: morphology and particle size.

Application Studies

Depending on framework functionality:

- **Gas adsorption** (CO_2, H_2, CH_4).
- **Catalysis** (organic transformations or photocatalysis).
- **Adsorption of dyes/heavy metals** from water.
- **Sensing** (fluorescent or electrochemical).
- **Drug loading and release** (optional biomedical application).

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